Probability measure generated by the superfidelity

Zbigniew Puchała* and Jarosław Adam Miszczak†
Institute of Theoretical and Applied Informatics,
Polish Academy of Sciences, Bałtycka 5, 44-100 Gliwice, Poland
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We study the probability measure on the space of density matrices induced by the metric defined by using superfidelity. We give the formula for the probability density of eigenvalues. We also study some statistical properties of the set of density matrices equipped with the introduced measure and provide a method for generating density matrices according to the introduced measure.

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I. INTRODUCTION

Recent applications of quantum mechanics are based on processing and transferring information encoded in quantum states. Random quantum states can be used to study various effects unique to quantum information theory [1]. This is especially true if one needs to get some information about the typical properties of the system in question [2]. In many cases it is important to quantify to what degree states are similar to the average state or how, on average, given quantity evolves during the execution of a quantum procedure. The crucial question emerging in this situation is how one should choose random sample from the set of quantum states.

The aforementioned question be answered easily in the case of pure quantum states. In this situation there exists a single, natural measure for constructing ensembles of states, namely Fubini-Study measure. The situation is more complex in the case of mixed quantum states. The probability measure can be introduced using various distance measures between quantum states [2]. By choosing the metric we also choose the probability measure on the space of density matrices. Among the most commonly used metrics we can point out the trace distance, Hilbert-Schmidt distance, and Bures distance.

In the analysis of mixed quantum states Bures distance is the most commonly used metric among the ones mentioned above. It has many important properties [2]. In particular it is a Riemannian and monotone metric. On the space of pure states it reduces to Fubini-Study metric [3] and it induces the statistical distance in the subspace of diagonal density matrices [4].

The main aim of this paper is the analysis of the probability measure on the space of density matrices induced by the metric defined in terms of *superfidelity* [5]. We calculate the formula for the probability density of eigenvalues and study some properties of the space of quantum states equipped with the introduced measure. We also provide a method for sampling random density matrices according to the introduced distribution.

* z.puchala@iitis.pl
† miszczak@iitis.pl

This paper is organized as follows. In Section II we introduce notation and basic facts used in the following sections. In Section III we calculate the volume element for the measure generated by the metric based on superfidelity and compare it with the analogous metric based on quantum fidelity. In Section IV we provide a formula for a probability density function on a simplex of eigenvalues. We also calculate the normalization constant in the low-dimensional case. In Section V we provide a method for sampling density matrices according to the introduced measure. Finally, in Section VI we provide a summary of the presented results.

II. PRELIMINARIES

Let use denote by $\mathcal{M}_N$ the space of density matrices of size N, *i.e.* $N \times N$ positive matrices with unit trace. By Δ we denote the simplex of eigenvalues.

For two density matrices $\rho, \sigma \in \mathcal{M}_N$, Bures distance can be defined in terms of quantum fidelity [3] as

$$d_{\mathrm{B}}(\rho, \sigma) = \sqrt{2 - 2\sqrt{F(\rho, \sigma)}}, \tag{1}$$

where fidelity, $F(\rho, \sigma) = \left[\operatorname{tr} |\sqrt{\rho}\sqrt{\sigma}|\right]^2$, provides a measure of similarity on the space of density matrices.

Probability measure on the simplex of eigenvalues generated by Bures metric was calculated in [6–8]. Various statistical properties of ensembles of quantum states with respect to this measure were discussed in [9].

Bures distance is commonly used in quantum information theory as a natural metric on the space of density matrices. Unfortunately, fidelity used to express d_{B} has some serious drawbacks. In particular in order to calculate fidelity between two quantum states one needs to compute square root of matrix, which is in general computationally hard task. Also, fidelity cannot be measured directly in laboratory and thus cannot be used to analyse experiments directly.

These drawbacks motivated the introduction of a new measure of similarity, namely superfidelity [5], defined for $\rho, \sigma \in \mathcal{M}_N$ as

$$G(\rho, \sigma) = \operatorname{tr} \rho\sigma + \sqrt{1 - \operatorname{tr} \rho^2}\sqrt{1 - \operatorname{tr} \sigma^2}. \tag{2}$$

Superfidelity shares many features with fidelity, *i.e.* it is bounded, symmetric and unitarly invariant. Moreover it is jointly concave and supermultiplicative. It was proved that superfidelity gives an upper bound for fidelity, $F(\rho,\sigma) \leq G(\rho,\sigma)$, where the equality is for $\rho,\sigma \in \mathcal{M}_2$ or in the case where one of the states is pure. It was also shown that, although G is not monotone [10], it can be used to define metric on $\mathcal{M}_N$. Using the correspondence between quantum operations and quantum states, superfidelity can be used to introduce metric on the space of quantum channels [11]. Superfidelity was also proved to be useful in providing bounds on the trace distance [12] (*i.e.* distinguisabiliy of states [13]) and as a tool for studying new metrics on the space of quantum states [14].

In the following we use a metric on the space of density matrices defined for $\rho,\sigma \in \mathcal{M}_N$ as

$$d_G(\rho,\sigma) = \sqrt{2 - 2G(\rho,\sigma)}. \tag{3}$$

Before we discuss further properties of this metric we should stress that the direct analogous of the Bures distance, $d_{\sqrt{G}}(\rho,\sigma) = \sqrt{2 - 2\sqrt{G(\rho,\sigma)}}$, is not a metric. One should also note that, since G is not monotone it cannot be analysed using Morozova-Čencov-Petz theorem [2].

III. VOLUME ELEMENT FOR THE MEASURE

To obtain the probability measure induced by metric Eq. (3) one needs to derive the volume element.

The calculations below follow the approach used by Hübner [6]. We begin with the calculation of the line element

$$d_G^2(\rho,\rho+d\rho) = 2 - 2G(\rho,\rho+d\rho). \tag{4}$$

We introduce function $A(t) = G(\rho,\rho+td\rho)$, which allows to write the line element

$$g_{ij}d\rho^i d\rho^j = \frac{1}{2}\frac{d^2}{dt^2}[d_G^2(\rho,\rho+t\,d\rho)]\Big|_{t=0} \tag{5}$$

as

$$g_{ij}d\rho^i d\rho^j = -A''(t)\Big|_{t=0}. \tag{6}$$

Equivalently, with the use of matrix entries, the line element reads

$$g_{ij}d\rho^i d\rho^j = \frac{(\sum\lambda_i\langle i|d\rho|i\rangle)^2}{1-\sum\lambda_i^2} + \sum\langle i|(d\rho)^2|i\rangle. \tag{7}$$

Infinitesimal shift $\rho + d\rho$ can be decomposed as a shift in eigenvalues and infinitesimal unitary rotation [7]

$$\rho + d\rho = \rho + d\Lambda + [dU,\rho], \tag{8}$$

where $d\Lambda = \sum d\lambda_i|i\rangle\langle i|$ and $(dU)^\dagger = -dU$. Rewriting dU in computational basis gives

$$dU = \sum_{j,k}(dx_{jk} + \mathrm{i}dy_{jk})|j\rangle\langle k| \tag{9}$$

with real coefficients $dx_{jk} = -dx_{kj}$ and $dy_{jk} = dy_{kj}$. After some calculations one gets

$$\mathrm{tr}\,d\rho^2 = \sum_i(d\lambda_i)^2 + 2\sum_{i<j}(\lambda_i-\lambda_j)^2[(dx_{ij})^2 + (dy_{ij})^2] \tag{10}$$

and

$$\mathrm{tr}\,\rho d\rho = \sum_i \lambda_i d\lambda_i. \tag{11}$$

Expanding this we get the entries of the metric tensor

$$\begin{aligned} g_{ij}d\rho^i d\rho^j = &\sum_{i,j}\left(\frac{\lambda_i\lambda_j}{1-\mathrm{tr}\,\rho^2} + \delta_{ij}\right)d\lambda_i d\lambda_j \\ &+ 2\sum_{i<j}(\lambda_i-\lambda_j)^2[(dx_{ij})^2 + (dy_{ij})^2]. \end{aligned} \tag{12}$$

To obtain volume element of the sought measure, one must calculate the appropriate determinant

$$\begin{aligned} dV_G = &\sqrt{\det\left(\frac{\lambda_i\lambda_j}{1-\mathrm{tr}\,\rho^2} + \delta_{ij}\right)}d\lambda_1\ldots d\lambda_n \\ &\times\prod_{i<j}2(\lambda_i-\lambda_j)^2 dx_{ij}dy_{ij}. \end{aligned} \tag{13}$$

Using the equality

$$\det\left(\frac{\lambda_i\lambda_j}{1-\mathrm{tr}\,\rho^2} + \delta_{ij}\right) = 1 + \frac{\mathrm{tr}\,\rho^2}{1-\mathrm{tr}\,\rho^2} = \frac{1}{1-\mathrm{tr}\,\rho^2}, \tag{14}$$

we obtain the expression for the volume element

$$dV_G = \frac{d\lambda_1\ldots d\lambda_n}{\sqrt{1-\sum_i\lambda_i^2}}\prod_{i<j}2(\lambda_i-\lambda_j)^2 dx_{ij}dy_{ij}. \tag{15}$$

One can compare the above formulas for the line element with the analogous result for the metric given in terms of fidelity as

$$d_{B'}^2(\rho,\rho+d\rho) = 2\left(1 - F(\rho,\rho+d\rho)\right). \tag{16}$$

In this case it is easy to check that the line element is given by formula

$$d_{B'}^2(\rho,\rho+d\rho) = \sum_{ij}\frac{|\langle i|d\rho|j\rangle|^2}{\lambda_i+\lambda_j}. \tag{17}$$

In the one-qubit case the above formula reads

$$d_{B'}^2(\rho,\rho+d\rho) = \left(\frac{1}{2\lambda(1-\lambda)}\right)|d\rho_{11}|^2 + |d\rho_{12}|^2 + |d\rho_{21}|^2 \tag{18}$$

where λ and $1-\lambda$ are eigenvalues of ρ and $d\rho_{ij} = \langle i|d\rho|j\rangle$ and we have used the equality $\langle 1|d\rho|1\rangle = -\langle 2|d\rho|2\rangle$. This is identical to (7) for $N = 2$, which is what one expects since in this case $F(\rho,\sigma) = G(\rho,\sigma)$.

IV. PROBABILITY DENSITY FUNCTION

In order to obtain probability measure we need to specify the normalizing constant. This constant is an inverse of the integral of the volume element dV_G over the group of unitary matrices and over the simplex of eigenvalues.

A. Normalization constant

Integration with respect to $U(N)$ is independent from the integration over the simplex of eigenvalues. We can rewrite Eq. 15 as

$$dV_G = \left(\frac{2^{N(N-1)/2}}{\sqrt{1-\sum_i \lambda_i^2}} \prod_{i<j} (\lambda_i - \lambda_j)^2 \right) d\lambda_1 \ldots d\lambda_n \prod_{i \neq j} dx_{ij} dy_{ij}. \tag{19}$$

After integrating this formula over $U(N)$ we get

$$V_G = \Upsilon_N \int_\Delta \left(\frac{2^{N(N-1)/2}}{\sqrt{1-\sum_i \lambda_i^2}} \prod_{i<j} (\lambda_i - \lambda_j)^2 \right) d\lambda_1 \ldots d\lambda_n, \tag{20}$$

where Υ_N is the volume of projective $U(N)$ [4, Eq. (148)]

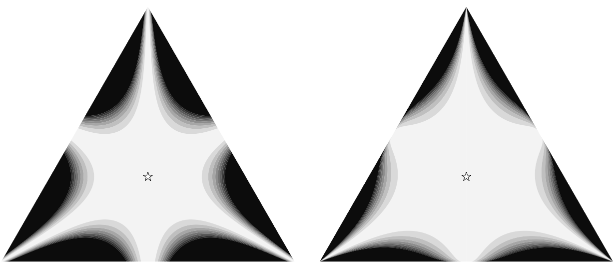
$$\Upsilon_N = \frac{\pi^{N(N-1)/2}}{\prod_{d=1}^{N-1} d!} \tag{21}$$

and Δ is the simplex of eigenvalues.

Probability density function on a simplex of eigenvalues is given by

$$f_{\mathrm{G},N}(\lambda) = C_N^{\mathrm{G}} \prod_{i<j} (\lambda_i - \lambda_j)^2 \frac{1}{\sqrt{1-\sum_i \lambda_i^2}}, \tag{22}$$

where C_N is a normalization constant. For $N=3$ function $f_{\mathrm{G},N}$ is presented in Fig. 1(a).



(a)Measure generated by $\sqrt{1-G}$ metric.

(b)Measure generated by the Bures metric

FIG. 1. Distribution of the eigenvalues for one-qutrit ($N=3$) density matrices for different probability measures.

The normalization constant C_N^{G} is the following integral

$$\frac{1}{C_N^{\mathrm{G}}} = \int_\Delta \prod_{i<j} (\lambda_i - \lambda_j)^2 \frac{1}{\sqrt{1-\sum_i \lambda_i^2}} d\lambda \tag{23}$$

over the simplex of eigenvalues.

The above integral can be written in terms of expectation value with respect to Hilbert-Schmidt measure

$$\frac{1}{C_N^{\mathrm{G}}} = \frac{1}{C_N^{\mathrm{HS}}} \mathrm{E}\left[\frac{1}{\sqrt{1-\mathrm{tr}\,\rho^2}} \right], \tag{24}$$

where ρ is a random state distributed with Hilbert-Schmidt measure and

$$C_N^{\mathrm{HS}} = \frac{\Gamma(N^2)}{\prod_{k=1}^N \Gamma(k)\Gamma(k+1)}. \tag{25}$$

The distribution of purity ($\mathrm{tr}\,\rho^2$) for random states is a subject of much study [15–17].

The probability distribution function of purity is known for Hilbert-Schmidt random states in the case of $N=2$ and $N=3$ [16]. Using these results, we can write explicitly normalizing constants

$$C_2^{\mathrm{G}} = \frac{2\sqrt{2}}{3\pi} C_2^{\mathrm{HS}}, \tag{26}$$

$$C_3^{\mathrm{G}} = \frac{432\sqrt{2}}{317\pi} C_3^{\mathrm{HS}}. \tag{27}$$

In the case of $N>3$ one can use the series expansion of $\frac{1}{\sqrt{1-r}}$ and rewrite the above as

$$\frac{1}{C_N^{\mathrm{G}}} = \frac{1}{C_N^{\mathrm{HS}}} \sum_{k=0}^{\infty} \frac{(2k-1)!!}{k! 2^k} \mathrm{E}[\mathrm{tr}\,(\rho^2)^k]. \tag{28}$$

The moments of purity for Hilbert-Schmidt random state are given by [15, 16]

$$\mathrm{E}[(\mathrm{tr}\,\rho^2)^k] = \frac{N!(N^2-1)!}{(N^2+2N-1)!} \sum_{k_1+\cdots+k_N=k} \frac{k!}{\prod_{i=1}^N k_i!} \times \prod_{i=1}^n \frac{(n+2k_i-i)!}{(q-i)! i!} \prod_{1 \le i<j \le n} (2k_i - i - 2k_j + j). \tag{29}$$

The constant C_N^{G} can be bounded from the above by using Jensen inequality

$$\frac{1}{C_N^{\mathrm{G}}} = \frac{1}{C_N^{\mathrm{HS}}} \mathrm{E}\left[\frac{1}{\sqrt{1-\mathrm{tr}\,\rho^2}} \right] \tag{30}$$

$$\ge \frac{1}{C_N^{\mathrm{HS}}} \frac{1}{\sqrt{1-E[\mathrm{tr}\,\rho^2]}} = \frac{1}{C_N^{\mathrm{HS}}} \frac{1}{\sqrt{1-\frac{2N}{N^2+1}}}, \tag{31}$$

thus

$$C_N^{\mathrm{G}} \le C_N^{\mathrm{HS}} \sqrt{1-\frac{2N}{N^2+1}}. \tag{32}$$

Since the distribution of purity has the variance given by

$$\sigma^2(\mathrm{tr}\,\rho^2) = \frac{2\left(N^2-1\right)^2}{\left(N^2+1\right)^2 \left(N^2+2\right)\left(N^2+3\right)}, \tag{33}$$

it tends to be more concentrated around the mean given by

$$\mathrm{E}[\mathrm{tr}\,\rho^2] = \frac{2N}{N^2+1}, \tag{34}$$

which tends to zero for large N. For small x, function $1/\sqrt{1-x}$ can be approximated with a small error by a linear function. Thus Jensen inequality gives good approximation of C_N^{G} for large values of N, where $\mathrm{tr}\,\rho^2$ tends to be small.

B. Mean purity

Let ρ_G be a random state distributed with measure G. Then the mean purity is given as

$$\mathrm{E}[\mathrm{tr}\,\rho_G^2] = \frac{C_N^{\mathrm{G}}}{C_N^{\mathrm{HS}}} \mathrm{E}\left[\frac{\mathrm{tr}\,\rho^2}{\sqrt{1-\mathrm{tr}\,\rho^2}}\right], \tag{35}$$

where ρ has Hilbert-Schmidt distribution. Next we have

$$\mathrm{E}\left[\frac{\mathrm{tr}\,\rho^2}{\sqrt{1-\mathrm{tr}\,\rho^2}}\right] \geq \mathrm{E}\left[\mathrm{tr}\,\rho^2\right] \mathrm{E}\left[\frac{1}{\sqrt{1-\mathrm{tr}\,\rho^2}}\right], \tag{36}$$

which follows from the fact that random variables $\mathrm{tr}\,\rho^2$ and $\frac{1}{\sqrt{1-\mathrm{tr}\,\rho^2}}$ are associated (see *e.g.* [18]). Finally, by using Eq. (24), we get

$$\mathrm{E}[\mathrm{tr}\,\rho_G^2] \geq \frac{C_N^{\mathrm{G}}}{C_N^{\mathrm{HS}}} \mathrm{E}\left[\mathrm{tr}\,\rho^2\right] \mathrm{E}\left[\frac{1}{\sqrt{1-\mathrm{tr}\,\rho^2}}\right] = \mathrm{E}\left[\mathrm{tr}\,\rho^2\right]. \tag{37}$$

From the above one can see that the mean purity for random state distributed with measure induced by the superfidelity is greater than the mean purity for random state distributed with Hilbert-Schmidt distribution.

V. GENERATING RANDOM STATES

A. One qubit case

In the case of 2×2 matrices the density function on the simplex of eigenvalues reads

$$f_{\mathrm{G},2}(\lambda, 1-\lambda) = \frac{2\sqrt{2}}{\pi} \frac{1}{\sqrt{\lambda(1-\lambda)}}. \tag{38}$$

Then the cumulative probability function for eigenvalues by integrating $f_{G,2}$ over interval $[0, t]$ reads

$$F_{\mathrm{G},2}(t) = \frac{2}{\pi}\left(\sqrt{(1-t)t} - 2\sqrt{(1-t)t^3} + \arcsin\sqrt{t}\right) \tag{39}$$

From the above we obtain a simple method for generating matrices with the above distribution. First one must generate eigenvalues of the matrix by inverting the cumulative distribution function and then rotate it by a random unitary matrix distributed with respect to Haar measure.

B. General case

To generate random state of dimension $N > 2$ distributed with measure induced by the superfidelity, one can use the rejection method (see *e.g.* [19]).

Probability density function $f_{\mathrm{G},N}$ on a simplex of eigenvalues can be bounded as

$$f_{\mathrm{G},N}(\lambda) \leq c f_{\mathrm{B},N}(\lambda), \quad \forall \lambda \in \Delta \tag{40}$$

where $f_{\mathrm{B},N}$ is a probability density function generated by Bures measure [2] (see Fig. 1(b))

$$f_{\mathrm{B},N}(\lambda) = C_N^{\mathrm{B}} \frac{1}{\sqrt{\lambda_1 \ldots \lambda_N}} \prod_{i<j} \frac{(\lambda_i - \lambda_j)^2}{\lambda_i + \lambda_j}. \tag{41}$$

Indeed, we have

$$\sup_{\lambda} \frac{f_{\mathrm{G},N}(\lambda)}{f_{\mathrm{B},N}(\lambda)} = \frac{C_N^{\mathrm{G}}}{C_N^{\mathrm{B}}} \frac{N^{-N/2}(2/N)^{N(N-1)/2}}{\sqrt{1-1/N}} \tag{42}$$

and using the bound for C_N^{G} one can take

$$c = \frac{\sqrt{\frac{N^2-N}{N^2+1}}\Gamma(N^2)\pi^{N/2}}{\prod_{i=1}^{N}\Gamma(i)2^{N(N-1)/2}\Gamma(N^2/2)N^{N^2/2}} \tag{43}$$

as the constant in Eq. (40).

In order to generate a matrix distributed according to the measure induced by the superfidelity, one needs to generate a random matrix X distributed with Bures measure [20] and a random number u distributed uniformly over the unit interval $[0, 1]$. To accept X as a matrix distributed according to the measure induced by the superfidelity, we check if $u \leq \frac{1}{c}\frac{f_{\mathrm{G},N}(X)}{f_{\mathrm{B},N}(X)}$ holds. Unfortunately, constant c increases very rapidly with N and thus this method does not work very efficiently for large N.

VI. SUMMARY

We have analysed random density matrices distributed according to probability measure induced by superfildelity. We have derived the formula for the probability density of eigenvalues according to this measure. We have also shown that random states distributed according to this measure have mean purity larger than in the case of Hilbert-Schmidt measure. We also provide a method for generating random matrices according to the introduced distribution.

Still there are some problems which require further investigations. The first is the calculation of the exact formula for the normalization constant for the probability density function. This is directly related to the distribution of purity for measures induced by the partial trace [15, 16]. The second problem is the inefficient method of sampling random states with the introduced measure, which could be used for numerical studies of the geometry of quantum states [2, 21, 22].

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